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HIGH TEMPERATURE HEAT CAPACITY EQUATIONS AND THERMODYNAMIC PROPERTIES OF COMBUSTION GASES

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ABSTRACT. This report contains the standard state heat of formation, reference enthalpy, reference entropy, and heat capacity equations for 200 chemical compounds. These compounds are those experimentally shown to exist and those theorized as existing in high temperature combustion processes. Thermodynamic data are given for compounds consisting of the following chemical elements: hydrogen, oxygen, nitrogen, carbon, lithium, sodium potassium, rubidium, cesium, magnesium, aluminum, fluorine, chlorine, bromine, beryllium, boron, silicon, and calcium.

The temperature range covered in most cases is 500°K to 6000°K, for which two heat capacity equations were derived of the form $C_P = a + bT + cT^{-2}$. One equation is given for the low temperature range, and another for the high temperature range. In the case of different physical states occurring in this range (solid → liquid → gas), one equation is normally given for each non-gas and two for each gas.

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INTRODUCTION

In the solution of high temperature combustion problems, such as the determination of flame temperature, the consideration of a large number of chemical elements and thus a large number of combustion products, results in the accumulation of large stacks of thermodynamic tables. Besides the large computer storage required, the seemingly endless interpolation of these data for an unlisted temperature or thermodynamic data point instigated a program for the condensation of these data into a more accessible and useful form. A heat capacity equation of the form

$$C_p = a + bT + cT^{-2}$$

was chosen, and a least square fit made of the changes in enthalpy as a function of temperature. For long temperature ranges, two heat capacity equations were derived. The fit error is most cases is quite small, and is sometimes better than the probable error in the original table. The fit is made in such a manner that errors, either typographical or proofreading, in the original data are detected and corrections or omissions may be made, i.e., we have checked the original data source for continuity. Thermodynamic data of this type should be a smooth continuous function except when phase changes occur. Another advantage of the use of an equation over tabulated data is that the number of entries to be proofread are minimized.

The majority of data presented in this report were completed by January 1960. The references used were restricted to those of an unclassified nature.

METHOD

Let us assume data are available showing enthalpy at various temperature intervals from T_1 to T_2, for which a heat capacity equation is to be derived ($C_p = (\partial H/\partial T)_p$). The enthalpy at $(T_1 + T_2)/2 = T_m$ is assumed to be a precise value, and the change in enthalpy with respect to temperature from T_m to all other tabulated data points in the range covered is computed. A least square fit is then made for C_p in the form of

$$C_p = a + bT + cT^{-2}$$

Instead of using the standard reference temperature of 298.15, a standard reference temperature (T^o) of 3000°K was chosen. (This should

not be confused with T_m although they may occasionally coincide). Each heat capacity equation derived was then used to compute an enthalpy (A), and an entropy (B), at 3000°K. The values A and B may be looked upon as integration constants from a standard reference temperature of 3000°K. This curve is assumed to be a continuous function and to pass through T^o at A. The value of A, and consequently B, may have no real significance, i.e., certain phases of a species may not exist at that temperature, or A and B may be grossly in error when compared to known enthalpy and entropy values at this temperature. A and B should be considered as working tools which enable one to obtain accurate values of enthalpy and entropy in the interval T_1 to T_2. It was for this reason that symbols other than H and S were chosen for these references. (For data tables where enthalpy is given at 3000°K, if this value is used instead of the A value, the average error incurred is increased by the amount $\Delta H_{298}^{3000} - A$). The enthalpy at temperature T_x may be computed as

$$\Delta H_{298.15}^{T_x} = A + \int_{3000}^{T_x} C_p dT$$

and the entropy at T_x as

$$S_{T_x} = B + \int_{3000}^{T_x} (C_p dT)/T$$

By adding the heat of formation $\Delta H_{f298.15}$ to the first equation, one may obtain the total enthalpy[1]

$$H^{T_x} = H_{f298.15} + A + \int_{3000}^{T_x} C_p dT$$

In the case of non-gas constituents the maximum temperature for the heat capacity equation is the melting point, or normal boiling point. The temperature range of a gaseous species is limited only by the data available. The reference enthalpy value, or integration constant A, may be somewhat more ambiguous when phase changes occur for a given species.

[1]The heat of formation was purposely maintained as a separate item since the uncertainty in this number is greater than that for other thermodynamic data, and other corrections will not be necessary if changes are made in $\Delta H_{f298.15}$.

For example, aluminum with a melting point of 900°K and a boiling point of 2710°K may follow the path

$$Al(s) + \Delta H_o^{T_f} + \Delta H_f = Al(l) \text{ at } T_f$$

$$Al(l) + \Delta H_f^{T_v} + \Delta H_v = Al(g) \text{ at } T_v$$

or we could assume aluminum gas at room temperature with a heat of formation:

$$\Delta H_{f298}\ Al(g) = \Delta H_{f298}\ Al(s) + \Delta H_f + \Delta H_v$$

and then heat the gas from room temperature to some temperature T_x. In one case the transition enthalpies have been used as corrections to the heat of formation, and in the other case they have been used as corrections to the changes in enthalpy. The same heat of formation for the solid and liquid form of a compound is used and the transition enthalpy occurs at the melting point. This enables one to compute split phases at the melting point. With four exceptions the normal heat of formation of the gaseous form is used. These exceptions are Al, Li, Na, and Mg gaseous atoms whose heat of formation are taken as zero.

Table 1 contains the constants A, B, a, b, c, the upper temperature limit (T_u) and the lower temperature limit (T_l) of the temperature interval over which the heat capacity equation was derived.

The accuracy of the fitted equation to the given tabular data is shown in Table 2, as a function of the given enthalpy (H_g), the given entropy (S_g), and the computed enthalpy (H_c), and the computed entropy (S_c). The error in enthalpy (E_h) and the error in entropy (E_s) are thus computed as

$$E_h = \frac{(H_g - H_c)100}{H_c}$$

$$E_s = \frac{(S_g - S_c)100}{S_c}$$

The maximum values of E_h and E_s, and the temperature at which each maximum occurred, are given for each heat capacity equation of Table 2. The fit error in most cases is quite small, and is frequently better than the probable error in the original data.

TABLE 1. Constants For the Computation of the High Temperature Heat Capacity, Enthalpy and Entropy of Combustion Products

Note: The constants A, B, a, b, c are given in IBM format. The number is given to 6 digits preceded by the sign of the number and an imaginary decimal point. The number is followed by the sign of the exponent and then the exponent. Thus /134219/5 is /.134219 x 10^5 or /13421.9 and /564739-4 is /.0000564739. Phase 1 = gas Phase 2 = solid Phase 3 = liquid

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
H	1	+134219+5	+496913+1	-714522-6	-282708+3	+388625+2	500	3000	1
	1	+134223+5	+496717+1	+202902-6	-172533+4	+388627+2	3000	6000	
H_2	1	+212345+5	+642855+1	+864880-3	-250591+5	+484762+2	500	3000	1
	1	+212474+5	+876781+1	+252545-3	-700794+7	+484814+2	3000	6000	
H_2O	1	+302726+5	+918719+1	+154169-2	-692461+6	+684367+2	500	3000	1
	1	+302359+5	+196232+2	-856621-3	-366959+8	+684340+2	3000	6000	
OH	1	+214857+5	+680978+1	+742330-3	-143735+6	+613842+2	500	3000	1
	1	+214589+5	+8583 9+1	+211153-3	-353053+7	+613791+2	3000	6000	
N	1	+134344+5	+494684+1	+122082-4	+665158+4	+480893+2	400	3100	4
	1	+134312+5	+221818+1	+604571-3	+918672+7	+480882+2	3100	6000	
N_2	1	+221820+5	+797126+1	+349537-3	-428312+6	+637631+2	500	3000	1
	1	+221610+5	+901527+1	+324151-4	-246855+7	+637532+2	3000	6000	
NO	1	+227519+5	+801039+1	+377348-3	-154347+6	+688615+2	500	3000	1
	1	+227211+5	+873566+1	+96 566-4	-242472+6	+688524+2	3000	6000	
NO_2	1	+382491+5	+105130+2	+238926-2	-279960+6	+867589+2	500	1100	1
	1	+348732+5	+134375+2	+277591-3	-152953+7	+852256+2	1100	2000	

NH_3	1	+476249+5	+678258+1	+657373-2	+213805+5	+793627+2	500	1500	1
	1	+412224+5	+187814+2	-534284-4	-606657+7	+766165+2	1500	3100	
NH	1	+217972+5	+718216+1	+654812-3	-275581+6	+609364+2	500	3000	1
	1	+217662+5	+888636+1	+124445-3	-294026+7	+609280+2	3000	6000	
HF	1	+211079+5	+658280+1	+766502-3	-765521+5	+587279+2	500	3000	1
	1	+210755+5	+762444+1	+342775-3	+726549+6	+587080+2	3000	6000	
HCl	1	+218936+5	+742795+1	+558871-3	-335299+6	+623709+2	500	3000	1
	1	+218653+5	+8903 5+1	+932206-4	-254887+7	+623640+2	3000	6000	
HBr	1	+222042+5	+773182+1	+479703-3	-39819+6	+654189+2	500	3000	1
	1	+221793+5	+890938+1	+10 84-3	-202848+7	+654130+2	3000	6000	
HI	1	+227096+5	+7655 5+1	+607342-3	-30842+6	+676304+2	500	2300	8
	1	+225358+5	+835281+1	+226927-3	+334420+6	+675665+2	2300	6000	
O	1	+135186+5	+495165+1	+10 159-4	+351743+5	+500939+2	500	3000	1
	1	+135226+5	+455392+1	+127018-3	+513186+6	+500952+2	3000	6000	
O_2	1	+234447+5	+812927+1	+485368-3	-275743+6	+679798+2	500	3000	1
	1	+234489+5	+102348+2	+457380-4	-773465+7	+679813+2	3000	6000	
Cl	1	+140188+5	+528947+1	-101964-3	+101290+6	+516206+2	500	3000	3
	1	+140261+5	+497353+1	-34 596-6	+553423+6	+516228+2	3000	6000	
Cl_2	1	+244164+5	+893571+1	+123693-3	-976482+5	+737624+2	500	3000	3
	1	+244165+5	+893763+1	+122413-3	-855418+5	+737621+2	3000	6000	
F	1	+136811+5	+501117+1	-144929-4	+817115+5	+497905+2	500	3000	1
	1	+136824+5	+496779+1	+986247-7	+138242+6	+497903+2	3000	6000	
F_2	1	+242516+5	+888624+1	+184982-3	-218745+6	+684627+2	500	3000	1
	1	+242503+5	+893677+1	+166914-3	-254764+6	+684639+2	3000	6000	
I	1	+136798+5	+471569+1	+179940-3	+625294+5	+547646+2	500	2500	10
	1	+137016+5	+568160+1	-228792-4	-275377+7	+547724+2	2500	5000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
I_2	1	+247022+5	+894199+1	+131651-3	-143111+5	+832017+2	500	1500	10
	1	+247059+5	+900034+1	+112730-3	-746383+5	+832039+2	1500	3000	
Br_2	1	+245192+5	+893573+1	+106527-3	-326941+5	+793851+2	500	2500	1
	1	+245181+5	+895534+1	+10 647-3	-706248+5	+793852+2	2500	4500	
IF	1	+248157+5	+882350+1	+275585-3	-800052+5	+770990+2	500	2500	8
	1	+248894+5	+657255+1	+117741-2	-15208+7	+771270+2	2500	6000	
ClF	1	+241214+5	+891283+1	+114714-3	-172582+6	+721315+2	500	3000	3
	1	+241208+5	+894445+1	+104563-3	-213105+6	+721321+2	3000	6000	
ClO	1	+241010+5	+889924+1	+134711-3	-202588+6	+727336+2	500	3000	3
	1	+241002+5	+893445+1	+121780-3	-223817+6	+727326+2	3000	6000	
ONF	1	+352626+5	+131499+2	+29 224-3	-623046+6	+878433+2	500	2500	1
	1	+351792+5	+1391 2+2	-697543-6	-138930+7	+878134+2	2500	5000	
C	2	+146485+5	+578587+1	+115385-3	-700661+6	+121340+2	500	4000	12
	2	+146485+5	+578587+1	+115385-3	-700661+6	+121340+2	500	4000	
C	1	+135409+5	+478746+1	+109074-3	+577426+5	+492851+2	500	3000	1
	1	+135516+5	+543044+1	+34 335-4	-352564+7	+492889+2	3000	6000	
CO	1	+223754+5	+813878+1	+302427-3	-441544+6	+653758+2	500	3000	1
	1	+223561+5	+887928+1	+548161-4	-133563+7	+653698+2	3000	6000	
CO_2	1	+365606+5	+136291+2	+504544-3	-104589+7	+798472+2	500	3000	1
	1	+365147+5	+121212+2	+58 07-3	+104398+8	+798350+2	3000	6000	

C_2	1	+229752+5	+856212+1	+183458-3	-417122+6	+680077+2	500	3000	1
	1	+229790+5	+633866+1	+228455-3	-106257+7	+680131+2	3000	6000	
C_3	1	+374188+5	+1416 1+2	+246384-3	-800596+6	+853969+2	500	3000	1
	1	+374003+5	+149166+2	-241697-5	-182563+7	+853917+2	3000	6000	
CH	1	+219918+5	+7148 6+1	+687220-3	-216113+6	+601197+2	500	3000	1
	1	+219527+5	+890886+1	+117306-3	-266297+7	+601100+2	3000	6000	
CH_2	1	+310321+5	+105733+2	+104360-2	-102342+7	+689043+2	500	3000	1
	1	+309673+5	+138319+2	+938800-5	-581348+7	+688880+2	3000	6000	
CH_3	1	+429528+5	+115620+2	+328539-2	-127486+7	+769866+2	500	2100	11
	1	+415443+5	+195949+2	+387540-4	-923326+7	+764519+2	2100	6000	
CH_4	1	+536247+5	+199055+2	+199409-2	-496670+7	+828268+2	1100	1900	1
	1	+530962+5	+251450+2	+117678-3	-113829+8	+826259+2	1900	4500	
C_2H_2	1	+505104+5	+1178 1+2	+435128-2	-223447+6	+856382+2	500	1800	1
	1	+471220+5	+202440+2	+11 976-3	-603852+7	+844088+2	1800	3100	
C_2H_4	1	+763725+5	+149798+2	+872879-2	-111586+7	+105480+3	500	1000	1
	1	+692813+5	+226738+2	+352321-2	-359846+7	+102408+3	1000	1500	
HCO	1	+32367+5	+1143 9+2	+768535-3	-869533+6	+794276+2	500	3000	1
	1	+323206+5	+138440+2	+795168-5	-449379+7	+794155+2	3000	6000	
CH_2O	1	+520408+5	+863569+1	+668099-2	-40442+6	+884835+2	500	1000	1
	1	+476391+5	+553380+1	+645717-2	-366033+7	+864711+2	1000	1500	
F_2CO	1	+491852+5	+186872+2	+452705-3	-129766+7	+100637+3	500	2500	1
	1	+490556+5	+196598+2	+125534-5	-243434+7	+100585+3	2500	5000	
HCN	1	+360111+5	+105440+2	+194341-2	-448416+6	+759397+2	500	1800	1
	1	+349109+5	+149715+2	+154825-4	-428453+7	+755162+2	1800	3000	
CN	1	+232350+5	+716072+1	+943966-3	-12798+6	+669730+2	500	3000	1
	1	+232551+5	+129640+2	-222507-3	-209829+8	+669779+2	3000	6000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
C_2N_2	1	+513932+5	+185046+2	+896547-3	-107859+7	+988315+2	500	2500	1
	1	+511095+5	+2093 +2	-219701-4	-375420+7	+987299+2	2500	4500	
CF	1	+234572+5	+875177+1	+145001-3	-340008+6	+701240+2	500	3000	1
	1	+234497+5	+885346+1	+90 829-4	-591129+5	+701169+2	3000	5500	
CF_2	1	+351473+5	+135328+2	+128891-3	-779766+6	+856706+2	500	3000	1
	1	+35131+5	+123376+2	+267221-3	+647196+7	+856569+2	3000	5500	
CF_3	1	+498801+5	+193317+2	+183065-3	-123804+7	+102173+3	500	3000	1
	1	+498679+5	+188530+2	+18 680-3	+257562+7	+102165+3	3000	5500	
CF_4	1	+645760+5	+253890+2	+139463-3	-18110+7	+113838+3	500	3000	1
	1	+644938+5	+1777 1+2	+134631-2	+389524+8	+113813+3	3000	5500	
C_2F_2	1	+580731+5	+199054+2	+154141-2	-10467+7	+10629+3	500	3000	1
	1	+580609+5	+217910+2	+106928-2	-694876+7	+106295+3	3000	5500	
CHF_3	1	+613822+5	+227146+2	+113374-2	-200112+7	+109168+3	500	2500	1
	1	+610900+5	+257472+2	+116028-4	-536512+7	+109064+3	2500	4500	
CH_2F_2	1	+583972+5	+205987+2	+189002-2	-233607+7	+102417+3	500	2500	1
	1	+57919+5	+256129+2	+342310-4	-782284+7	+102240+3	2500	4500	
CH_3F	1	+558845+5	+186130+2	+259363-2	-252186+	+937897+2	500	2500	1
	1	+552375+5	+255520+2	+419789-4	-102832+8	+935617+2	2500	4500	

FCN	1	+371737+5	+135899+2	+489249-3	-703130+6	+838515+2	500	2500	1
	1	+370409+5	+148746+2	+429504-5	-204248+7	+838051+2	2500	5000	
Cl_2CO	1	+514379+5	+184063+2	+727195-3	-545130+6	+110923+3	400	1600	8
	1	+508688+5	+198723+2	-959135-5	-136626+7	+110712+3	1600	5000	
CCl	1	+238841+5	+8788 8+1	+122476-3	-14661 6+6	+737904+2	500	1400	8
	1	+237840+5	+894391+1	+317184-4	-224338+6	+737483+2	1400	6000	
CCl_4	1	+678391+5	+255880+2	+11 797-3	-61629+6	+130476+3	400	2000	8
	1	+678391+5	+255880+2	+11 797-3	-61629+6	+130476+3	400	2000	
FClCO	1	+529967+5	+164859+2	+225299-2	-550313+6	+107556+3	400	1100	8
	1	+498599+5	+197751+2	+198544-4	-174799+7	+106184+3	1100	4500	
Be	2	+21728 4+5	+420018+1	+235639-2	-11285 4+5	+180521+2	500	1556	2
	3	+215499+5	+750257+1	-808379-6	-367640+4	+186150+2	1556	2700	
Be	1	+134242+5	+496932+1	+383367-6	-392597+3	+440189+2	500	3000	2
	1	+134226+5	-1659 +1	+138584-2	+237650+8	+440104+2	3000	6000	
BeO	1	+231901+5	+866229+1	+161855-3	-390569+6	+661436+2	500	3000	3
	1	+231829+5	+894243+1	+681567-4	-737726+6	+661427+2	3000	6000	
BeO	2	+355146+5	+104899+2	+198427-2	-585171+6	+299903+2	500	2823	2
	3	+494900+5	+1600 +2	+00		+349471+2	2823	5000	
Be_2O_2	1	+492953+5	+189779+2	+362734-3	-138382+7	+972840+2	500	2500	13
	1	+491623+5	+198663+2	+918709-6	+216126+7	+972373+2	2500	6000	
Be_3O_3	1	+781225+5	+310978+2	+208380-3	-265956+7	+125141+3	500	3700	13
	1	+781388+5	+317919+2	+298456-6	-361810+7	+125149+3	3700	6000	
BeO_2H_2	1	+598557+5	+182763+2	+335409-2	-179813+7	+971703+2	500	2100	13
	1	+583242+5	+264542+2	+516234-4	-103576+8	+965817+2	2100	6000	
BeCl	1	+239972+5	+889776+1	+107614-3	-193600+6	+719242+2	500	3000	3
	1	+239957+5	+894767+1	+911253-4	-268438+6	+719246+2	3000	6000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
$BeCl_2$	3	+562500+5	+2000 +2	+00		+688051+2	700	1000	2
	3	+562500+5	+2000 +2	+00		+688051+2	700	1000	
$BeCl_2$	1	+388115+5	+1480 1+2	+31 497-4	-486442+6	+898595+2	500	3000	2
	1	+38808+5	+147731+2	+192207-4	+123651+6	+89857+2	3000	6000	
Be_2Cl_4	1	+793486+5	+312181+2	+18 619-3	-22754+7	+128648+3	500	3500	13
	1	+793543+5	+3180 4+2	-971230-6	-299949+7	+128345+3	3500	6000	
BeFCl	1	+38033+5	+1469 5+2	+731184-4	-745493+6	+866514+2	500	3000	4
	1	+380274+5	+149315+2	-429443-5	-113988+7	+866534+2	3000	6000	
BeF	1	+234717+5	+877051+1	+135857-3	-33650+6	+684033+2	500	3000	3
	1	+234670+5	+894430+1	+771963-4	-546270+6	+684025+2	3000	6000	
BeF_2	2	+761690+5	+839582+1	+12 42-1	+580358+3	+608186+2	500	0820	2
	3	+566558+5	+210078+2	-438064-5	-354621+4	+54660+2	820	1500	
BeF_2	1	+374219+5	+144654+2	+15 234-3	-896657+6	+822010+2	500	3000	2
	1	+374583+5	+196062+2	-703529-3	-297020+8	+82212+2	3000	6000	
BeH	1	+22942+5	+821629+1	+385306-3	-435813+6	+607264+2	500	3000	2
	1	+229210+5	+895287+1	+139425-3	-139118+7	+607137+2	3000	6000	
Be_3N_2	2	+916757+5	+326471+2	+244364-2	-302742+7	+817701+2	500	2470	12
	3	+121876+6	+489054+2	-40 116-2	-159661+5	+94077+2	2470	4000	
Be_2C	2	+529278+5	+166211+2	+267002-2	-166180+7	+434200+2	500	2400	12
	3	+702540+5	+292089+2	-241115-2	-135710+6	+506886+2	2400	3500	

Na	3	+109499+5	+101529+2	-366974-2	-280371+6	+261293+2	500	0800	2
	3	+250387+5	+194810+1	+366803-2	+132054+7	+325901+2	800	1100	
Na	1	+393669+5	+433987+1	+227685-3	+649205+6	+482053+2	1200	3600	2
	1	+391464+5	-573373+1	+207871-2	+475343+8	+481340+2	3600	6000	
Na_2	1	+259835+5	+875773+1	+477366-3	+644089+5	+767039+2	500	3500	8
	1	+258960+5	+624287+1	+106556-2	+661883+7	+760294+2	3500	6000	
Na_2O	2	+674060+5	+150938+2	+591992-2	+102899+6	+686589+2	500	1190	2
	3	+710198+5	+240027+2	-984430-6	-269295+4	+745397+2	1190	2500	
NaO	1	+243163+5	+892748+1	+133128-3	-131593+6	+743818+2	500	3400	8
	1	+243460+5	+892339+1	+131144-3	-203878+5	+743815+2	3400	6000	
NaOH	3	+560743+5	+196656+2	+594817-4	+337805+6	+644439+2	600	1300	2
	3	+562800+5	+2000 +2	+00		+645422+2	1300	2000	
NaOH	1	+331751+5	+116478+2	+678813-3	-572650+6	+779180+2	500	3000	2
	1	+331358+5	+138328+2	+648489-5	-397347+7	+779042+2	3000	6000	
NaH	1	+242501+5	+8853 5+1	+255744-3	-315541+6	+647281+2	500	3000	2
	1	+242448+5	+907747+1	+203250-3	-111828+7	+647290+2	3000	6000	
NaCl	2	+472689+5	+1090 6+2	+399941-2	-102272+3	+533021+2	500	1081	2
	3	+482400+5	+1600 +2	+00		+571704+2	1081	2000	
NaCl	1	+248007+5	+898090+1	+162970-3	-705863+5	+757263+2	500	3000	2
	1	+24799+5	+8932521	+179343-3	+117308+6	+757255+2	3000	6000	
NaF	2	+452308+5	+104791+2	+383186-2	-549750+5	+465510+2	500	1285	2
	3	+493595+5	+164052+2	-195231-5	-527268+4	+512574+2	1285	2300	
NaF	1	+246371+5	+897520+1	+141056-3	-872266+5	+730154+2	500	3000	2
	1	+246411+5	+904845+1	+138463-3	-563877+6	+730209+2	3000	6000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
Al	1	+909582+5	+484945+1	+371123-4	-240878+5	+508440+2	2800	4400	2
	1	+905307+5	-235160+0	+801207-3	+338221+8	+507131+2	4400	6000	
Al	3	+213300+5	+7000 +1	+00		+252150+2	1000	1800	2
	3	+213299+5	+700716+1	-214274-5	-114764+5	+252110+2	1800	2700	
AlH	1	+233962+5	+858053+1	+276733-3	-43829?+6	+637919+2	500	3000	2
	1	+233907+5	+895658+1	+16 561-3	-106893+7	+637906+2	3000	6000	
AlO	1	+238056+5	+887332+1	+104638-3	-241789+6	+718594+2	500	3000	3
	1	+238042+5	+894543+1	+81 514-4	-344072+6	+718590+2	3000	6000	
Al_2O	1	+35249+5	+135162+2	+129835-3	-737678+6	+890873+2	500	3000	2
	1	+352444+5	+138932+2	+853550-6	-116093+7	+890813+2	3000	6000	
Al_2O_2	1	+536813+5	+205726+2	+982899-4	-890923+6	+105431+3	500	3000	4
	1	+536744+5	+208573+2	+153325-5	-121348+7	+105428+3	3000	6000	
Al_2O_3	2	+851343+5	+276426+2	+294620-2	-851733+6	+789515+2	500	2310	2
	3	+110910+6	+350063+2	-114715-5	-258244+5	+901698+2	2310	5000	
AlOH	1	+367485+5	+143427+2	+189182-3	-112680+7	+803553+2	500	3000	4
	1	+367335+5	+1491 3+2	-116219-5	-183316+7	+803587+2	3000	6000	
AlO_2H	1	+480886+5	+177152+2	+66 657-3	-110173+7	+989874+2	500	3000	4
	1	+480500+5	+197817+2	+12 515-4	-421171+7	+989811+2	3000	6000	
AlOCl	1	+392010+5	+148420+2	+215132-4	-358935+6	+920500+2	500	3000	4
	1	+391996+5	+148865+2	+308478-5	-353481+6	+920413+2	3000	6000	

AlOF	1	+386927+5	+148129+2	+312106-4	-532534+6	+876977+2	500	3000	4
	1	+386905+5	+149094+2	-502102-6	-694215+6	+876959+2	3000	6000	
AlCl	1	+244670+5	+893787+1	+119075-3	-734761+5	+750363+2	500	3000	3
	1	+244667+5	+895621+1	+115215-3	-144776+6	+750372+2	3000	6000	
$AlCl_2$	1	+371171+5	+138985+2	+409607-5	-157908+6	+994360+2	500	3000	4
	1	+371173+5	+139119+2	+958265-7	-202536+6	+994353+2	3000	6000	
$AlCl_3$	3	+915810+5	+312010+2	-703074-6	-240863+3	+109408+3	465	1400	4
	3	+915810+5	+312010+2	-703074-6	-240863+3	+109408+3	465	1400	
$AlCl_3$	1	+527961+5	+198615+2	+209913-6	-307158+6	+120056+3	500	3000	2
	1	+527954+5	+199037+2	-21 669-5	-802343+6	+120048+3	3000	6000	
Al_2Cl_6	1	+143154+6	+434866+2	+849664-4	-572391+6	+207509+3	500	0900	2
	1	+152826+6	+310581+2	+796349-2	+393857+7	+211630+3	900	1200	
AlF	1	+240344+5	+890348+1	+103296-3	-176629+6	+713966+2	500	3000	3
	1	+240332+5	+894413+1	+892936-4	-240054+6	+713969+2	3000	6000	
AlF_2	1	+365129+5	+137837+2	+589820-4	-353435+6	+930719+2	500	2000	8
	1	+364762+5	+1391 1+2	-152817-6	-436271+6	+930582+2	2000	4500	
$AlFCl_2$	1	+524999+5	+198251+2	+161644-4	-402868+6	+117327+3	500	3000	4
	1	+524984+5	+198687+2	+453697-6	-425035+6	+117836+3	3000	6000	
AlF_2Cl	1	+521363+5	+197950+2	+26 910-4	-526895+6	+114091+3	500	3000	4
	1	+521341+5	+198598+2	+17 923-5	-533023+6	+114091+3	3000	6000	
AlF_2	1	+364388+5	+138339+2	+264519-4	-386650+6	+919973+2	500	3000	4
	1	+364370+5	+139180+2	-972893-6	-529361+6	+919965+2	3000	6000	
AlF_2	2	+686981+5	+214935+2	+239838-2	+281358+6	+711348+2	500	1600	2
	2	+686981+5	+214935+2	+239838-2	+281358+6	+711348+2	500	1600	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
AlF_3	1	+520493+5	+197950+2	+234624-4	-550466+6	+109166+3	500	3000	4
	1	+520477+5	+199342+2	-103827-4	-905876+6	+109171+3	3000	6000	
ALi	1	+246519+5	+890821+1	+147176-3	-192953+5	+799662+2	500	3300	8
	1	+246205+5	+411327+1	+111600-2	+183966+8	+799559+2	3300	6000	
ALN	1	+241481+5	+879450+1	+193065-3	-170209+6	+743302+2	500	1500	8
	1	+240668+5	+880225+1	+144811-3	+639544+5	+742974+2	1500	6000	
ALN	2	+357617+5	+113851+2	+154007-2	-752088+6	+323663+2	500	2500	12
	2	+357617+5	+113851+2	+154007-2	-752088+6	+323663+2	500	2500	
B	2	+176002+5	+556825+1	+899820-3	-56783+6	+142702+2	500	2300	2
	3	+226300+5	+750084+1	-137728-6	-39624+4	+164724+2	2300	6000	
B	1	+134172+5	+498488+1	-807026-5	-61629+4	+481161+2	500	3000	2
	1	+134162+5	+430283+1	+124782-3	+285897+7	+481199+2	3000	6000	
B_2	1	+238216+5	+882855+1	+143565-3	-25271+6	+679072+2	500	3000	2
	1	+238194+5	+891048+1	+109181-3	-26329+6	+679015+2	3000	6000	
BH	1	+226762+5	+797846+1	+459472-3	-434357+6	+593351+2	500	3000	4
	1	+226555+5	+910080+1	+116574-3	-24313+7	+593261+2	3000	6000	
B_2O_3	1	+631773+5	+242389+2	+52 395-3	-188172+7	+115600+3	500	3000	2
	1	+631396+5	+255359+2	+517444-4	-274013+7	+115593+3	3000	6000	
B_2O_3	3	+838976+5	+305045+2	-251308-5	-19350+4	+817959+2	800	1600	2
	3	+838988+5	+305288+2	-948504-5	-38018+5	+817962+2	1600	2500	

BO	1	+226654+5	+841876+1	+213073-3	-453535+6	+670414+2	500	3000	2
	1	+226536+5	+892046+1	+465693-4	-113618+7	+670383+2	3000	6000	
B_2O_2	1	+520164+5	+197318+2	+348642-3	-119619+7	+101380+3	500	3000	2
	1	+520002+5	+206687+2	+358955-4	-220690+7	+101374+3	3000	6000	
HBO_2	1	+468681+5	+172219+2	+813461-3	-135429+7	+961998+2	500	3000	2
	1	+468224+5	+196040+2	+406831-4	-438479+7	+961856+2	3000	6000	
$H_2B_2O_4$	1	+946790+5	+454036+2	-818737-3	-772314+7	+150338+3	1400	2700	2
	1	+946790+5	+454036+2	-818737-3	-772314+7	+150338+3	2700	4000	
H_3BO_3	1	+823497+5	+292556+2	+218412-2	-268768+7	+130380+3	500	3000	2
	1	+822069+5	+350320+2	+183921-4	-358526+7	+130339+3	3000	6000	
BOCl	1	+378982+5	+142668+2	+225916-3	-702307+6	+876254+2	600	2700	13
	1	+378515+5	+148972+2	+829182-6	-144696+7	+876101+2	2700	6000	
BCl	1	+240032+5	+887453+1	+119748-3	-184794+6	+708788+2	500	3000	2
	1	+239999+5	+904772+1	+735109-4	-764824+6	+708748+2	3000	6000	
BCl_2	1	+363410+5	+137810+2	+50 69-4	-411482+5	+948167+2	500	2600	13
$BFCl_2$	1	+511743+5	+194993+2	+142784-3	-808841+6	+110484+3	500	2700	13
	1	+511370+5	+198663+2	+105400-5	-115280+7	+110472+3	2700	6000	
BCl_3	1	+517545+5	+197030+2	+601003-4	-640057+6	+111944+3	500	3000	2
	1	+517475+5	+1993 6+2	-972826-5	-115868+7	+111939+3	3000	6000	
BFCl	1	+357980+5	+135847+2	+124882-3	-562920+6	+923757+2	500	2700	13
	1	+357650+5	+139044+2	+109000-5	-862228+6	+923645+2	2700	6000	
BF	1	+232806+5	+871625+1	+143556-3	-370595+6	+669181+2	500	3000	2
	1	+232793+5	+898817+1	+651148-4	-880014+6	+669251+2	3000	6000	
BF_2	1	+349146+5	+132679+2	+231734-3	-790174+6	+868475+2	500	2700	13
	1	+348818+5	+139068+2	+431824-6	-145561+7	+868385+2	2700	6000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_I (°K)	T_U (°K)	Ref.
BF_3	1	+497268+5	+192551+2	+209201-3	-126812+7	+100352+3	500	3000	2
	1	+497104+5	+199822+2	-18 [illegible]4-4	-254074+7	+100383+3	3000	6000	
BF_2Cl	1	+504607+5	+192980+2	+217175-3	-101509+7	+106350+3	500	2700	13
	1	+504067+5	+198722+2	-217981-6	-158405+7	+106332+3	2700	6000	
BOF	1	+373228+5	+137542+2	+448045-3	-732207+6	+836684+2	500	2500	13
	1	+371721+5	+148924+2	+149312-5	-186303+7	+836140+2	2500	6000	
BBr	1	+241911+5	+891375+1	+109840-3	-136745+6	+739527+2	500	3000	4
	1	+241907+5	+897652+1	+958003-4	-366857+6	+739510+2	3000	6000	
BN	1	+231289+5	+860774+1	+182834-3	-391060+6	+691278+2	500	3000	2
	1	+230650+5	+627093+1	+475456-3	+151574+8	+691064+2	3000	6000	
BN	2	+379808+5	+574763+1	+519103-2	-214188+6	+296772+2	200	1678	5
	2	+379808+5	+574763+1	+519103-2	-214188+6	+296772+2	1678	3555	
Li	3	+192676+5	+671181+1	+606335-4	+107173+6	+240926+2	500	1500	2
	3	+192676+5	+671181+1	+606335-4	+107173+6	+240926+2	500	1500	
Li	1	+519590+5	+309019+1	+612590-3	+265138+7	+446539+2	1700	3800	2
	1	+514160+5	-895618+1	+261448-2	+700116+8	+444850+2	3800	6000	
Li_2	1	+249526+5	+8938 6+1	+206877-3	-400646+5	+680011+2	500	3000	3
	1	+249520+5	+894895+1	+203799-3	-794542+5	+680013+2	3000	6000	
LiC	1	+231950+5	+869083+1	+146589-3	-387681+6	+655971+2	500	3000	2
	1	+231879+5	+902512+1	+491713-4	-109989+7	+656008+2	3000	6000	

Li_2O	2	+665786+5	+147726+2	+619611-2	-301457+6	+581576+2	500	1700	2
	3	+737200+5	+2400 6+2	-162276-6	-123637+4	+636044+2	1700	3500	
Li_2O	1	+346209+5	+133253+2	+195712-3	-913976+6	+816515+2	500	3000	2
	1	+346077+5	+140418+2	-221018-4	-230510+7	+816408+2	3000	6000	
LiCH	3	+603546+5	+207413+2	-613881-6	-692181+3	+594206+2	800	2000	4
	3	+603546+5	+207413+2	-613881-6	-692181+3	+594206+2	800	2000	
LiCl	3	+459100+5	+1600 +2	+00		+525804+2	900	2000	4
	3	+459100+5	+1600 +2	+00		+525804+2	900	2000	
LiCl	1	+243781+5	+892885+1	+136293-3	-126362+6	+711942+2	500	3000	3
	1	+243779+5	+894893+1	+13 793-3	-170826+6	+711936+2	3000	6000	
Li_2Cl_2	1	+524978+5	+198345+2	+132515-4	-402654+6	+111408+3	500	3000	4
	1	+524968+5	+198777+2	-53 346-6	-492650+6	+111416+3	3000	6000	
LiF	2	+482242+5	+848089+1	+56 416-2	+164552+6	+437282+2	500	1200	3
	3	+460993+5	+155048+2	-192780-5	-416022+4	+458232+2	1200	2200	
LiF	1	+240659+5	+889290+1	+136827-3	-214228+6	+676758+2	500	3000	3
	1	+240648+5	+895618+1	+118128-3	-338321+6	+676758+2	3000	6000	
Li_2F_2	1	+515298+5	+1974 3+2	+454177-4	-729622+6	+103482+3	500	3000	4
	1	+515264+5	+198855+2	-172477-5	-973175+6	+103480+3	3000	6000	
LiH	1	+235371+5	+871383+1	+202566-3	-373187+6	+599675+2	500	3000	2
	1	+235319+5	+896789+1	+122803-3	-760475+6	+599631+2	3000	6000	
Li_2C_2	2	+744988+5	+243352+2	+244311-2	-706890+6	+728395+2	500	2000	12
	2	+744988+5	+243352+2	+244311-2	-706890+6	+728395+2	2000	2000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
Ca	1	+134866+5	+490769+1	+406131-4	+151838+5	+484854+2	500	2100	2
	1	+137490+5	-215150+1	+223467-2	+111486+8	+485879+2	2100	3000	
CaO	1	+247863+5	+867842+1	+336804-3	-536381+5	+751604+2	500	2800	8
	1	+247650+5	+9762 6+1	+167154-3	-483860+7	+751658+2	2800	6000	
CaCl	1	+245884+5	+887617+1	+152219-3	-237839+5	+784714+2	500	2700	8
	1	+245940+5	+592476+1	+908508-3	+695825+7	+784795+2	2700	5600	
CaF	1	+243225+5	+884590+1	+145772-3	-752302+5	+752382+2	500	3000	8
	1	+243180+5	+624074+1	+791034-3	+633395+7	+752412+2	3000	6000	
CaH	1	+238099+5	+858612+1	+328046-3	-281413+6	+677082+2	500	3100	8
	1	+239360+5	+845285+1	+501777-3	-395588+7	+677136+2	3100	6000	
Cs	1	+135681+5	+484829+1	+866756-4	+273435+5	+534671+2	500	1900	2
	1	+140250+5	-530783+0	+198086-2	+669612+7	+536502+2	1900	3000	
Cs_2	1	+274592+5	+826463+1	+101626-2	+199116+6	+902988+2	500	2800	8
	1	+273340+5	+113854+2	+665275-3	-170445+8	+903165+2	2800	6000	
CsCl	1	+250037+5	+894218+1	+199230-3	-146812+5	+823212+2	500	3400	8
	1	+250030+5	+893350+1	+20 558-3	+411679+5	+823213+2	3400	6000	
CsF	1	+252206+5	+894330+1	+254400-3	-252288+5	+797848+2	500	3300	8
	1	+252220+5	+891037+1	+259557-3	+181182+6	+797845+2	3300	6000	
CsH	1	+245361+5	+887012+1	+264159-3	-200806+6	+716573+2	500	3100	8
	1	+245990+5	+800759+1	+46 265-3	+234168+7	+716572+2	3100	6000	

Si	1	+138059+5	+479853+1	+151499-3	+642310+5	+519033+2	500	1400	2
	1	+140156+5	+567615+1	-168314-4	-158251+7	+519921+2	1400	6000	
Si	2	+187953+5	+543032+1	+974847-3	-682564+5	+192860+2	500	1683	2
	3	+289596+5	+700977+1	-166414-5	-418526+5	+255052+2	1683	6000	
Si_2	1	+242960+5	+892876+1	+995345-4	-899054+5	+763904+2	500	4500	8
	1	+243070+5	+106080+2	-907406-4	-173843+8	+785100+2	4500	6000	
SiO	1	+236504+5	+841858+1	+341293-3	-233144+6	+698614+2	500	1600	2
	1	+233672+5	+894372+1	+484269-4	-482843+6	+697372+2	1600	6000	
SiO_2	1	+385010+5	+138399+2	+615396-3	-607811+6	+848537+2	500	1400	2
	1	+378136+5	+146972+2	+54 141-6	-115685+7	+845674+2	1400	6000	
SiO_2	2	+474170+5	+146427+2	+182757-2	-126700+6	+475913+2	900	1883	2
	3	+482400+5	+180025+2	-565990-6	-656476+4	+482000+2	1883	6000	
SiCl	1	+244304+5	+893177+1	+974158-4	-449669+5	+774427+2	500	3400	8
	1	+346975+5	+800446+1	+273867-3	+392327+7	+774396+2	3400	6000	
SiF	1	+239415+5	+890142+1	+932176-4	-173502+6	+739685+2	500	3300	8
	1	+339170+5	+801283+1	+259673-3	+367834+7	+739658+2	3300	6000	
SiCl	1	+244304+5	+893177+1	+974158-4	-449669+5	+774427+2	500	3400	8
	1	+243070+5	+800446+1	+273867-3	+392327+7	+774396+2	3400	6000	
SiF	1	+239415+5	+890142+1	+932176-4	-173502+6	+739685+2	500	3300	8
	1	+240050+5	+801283+1	+259673-3	+367834+7	+739658+2	3300	6000	
$SiCl_2$	1	+369902+5	+139039+2	+169344-5	-193138+6	+980409+2	500	4500	8
	1	+370220+5	+175573+2	-464241-3	-330728+8	+102053+3	4500	6000	
$SiCl_4$	1	+683534+5	+258173+2	+411957-5	-469829+6	+136178+3	500	4500	8
	1	+684400+6	+325283+2	-851701-3	-609087+8	+143631+3	4500	6000	
SiF_4	1	+658470+5	+2569 1+2	+355945-4	-123222+7	+120637+3	500	4500	8
	1	+663390+6	+321424+2	-802334-3	-584600+8	+128227+3	4500	6000	

TABLE 1. (Contd.)

Species	Phase	A (cal/mole)	a (cal/°-mol)	b (cal/°-mol)	c (cal/°-mol)	B (cal/°-mol)	T_L (°K)	T_U (°K)	Ref.
K	1	+134793+5	-491875+1	+347325-4	+115351+5	+497875+2	500	2000	2
	1	+136480+5	-2204 1+1	+936751-3	+382657+7	+498571+2	2000	3000	
K_2	1	+265018+5	+8766 3+1	+596758-3	+524595+5	+816678+2	500	2800	8
	1	+264690+5	+928416+1	+601548-3	-418527+7	+816746+2	2800	6000	
KCl	1	+249247+5	+894096+1	+189809-3	-258281+5	+781210+2	500	3300	8
	1	+251490+5	+878695+1	+215288-3	+792608+6	+781201+2	3300	6000	
KF	1	+246681+5	+894019+1	+15 729-3	-524618+5	+749207+2	500	3100	8
	1	+246730+5	+895082+1	+148669-3	-100931+6	+749210+2	3100	6000	
KH	1	+243349+5	+8860 +1	+25 700-3	-238483+6	+673656+2	500	3100	8
	1	+244260+5	+799480+1	+43 811-3	+278692+7	+673650+2	3100	6000	
Rb	1	+134962+5	+490290+1	+454100-4	+155836+5	+521243+2	500	2000	2
	1	+136980+5	+178455+1	+109620 2	+423401+7	+522067+2	2000	3000	
Rb_2	1	+262571+5	+379610+1	+525822-3	+491953+5	+865854+2	500	3000	8
	1	+262160+5	+318934+1	+805667-3	-193177+7	+865910+2	3000	6000	
RbCl	1	+250197+5	+894336+1	+204576-3	-183295+5	+807927+2	500	3400	8
	1	+250210+5	+862933+1	+258074-3	+161788+7	+807904+2	3400	6000	
RbF	1	+247362+5	+889251+1	+172425-3	-192707+5	+775902+2	500	2900	8
	1	+247040+5	+914558+1	+118323-3	-139075+7	+775887+2	2900	6000	
RbH	1	+245008+5	+886656+1	+271059-3	-219463+6	+700592+2	500	3300	8
	1	+245770+5	+797316+1	+462385-3	+278122+7	+700583+2	3300	6000	

Mg	2	+293037+5	+463644+1	+346754-2	+255559+5	+280625+2	500	0923	4
	3	+291908+5	+527323+1	+26 789-2	+698532+3	+292953+2	923	2500	
Mg	1	+490414+5	+436613+1	+19 967-3	+836958+6	+469820+2	1400	3700	2
	1	+488548+5	-482896+1	+187928-2	+432386+8	+469131+2	3700	6000	
MgO	1	+240928+5	+891246+1	+108769-3	-173019+6	+709951+2	500	3000	3
	1	+240921+5	+895668+1	+964898-4	-277475+6	+709952+2	3000	6000	
MgO	2	+347738+5	+1023 6+2	+17 715-2	-155484+6	+339101+2	500	2200	2
	2	+348036+5	+100029+2	+177911-2	+322159+6	+339230+2	2200	4000	
$MgCl_2$	2	+600871+5	+188936+2	+143082-2	-206581+6	+677391+2	500	0987	4
	3	+712399+5	+221013+2	-499612-6	-114521+4	+789522+2	987	2500	
$MgCl_2$	1	+396781+5	+148940+2	+326829-5	-198618+6	+948625+2	500	3000	2
	1	+396774+5	+148083+2	+168655-4	+137661+6	+948662+2	3000	6000	
MgFCl	1	+393933+5	+148728+2	+116874-4	-292907+6	+924985+2	500	3000	4
	1	+393924+5	+148995+2	+974333-6	-312186+6	+924949+2	3000	6000	
MgF_2	2	+563585+5	+168667+2	+256816-2	-20636+6	+583246+2	500	1536	2
	3	+701900+5	+226055+2	-16 681-5	-892923+4	+674849+2	1536	3000	
MgF_2	1	+390723+5	+148285+2	-301721-4	-399428+6	+882615+2	500	3000	2
	1	+390676+5	+149586+2	-86 266-5	-783704+6	+882519+2	3000	6000	
MgH	1	+237354+5	+867887+1	+277050-3	-391929+6	+653771+2	500	3000	2
	1	+237298+5	+898875+1	+183462-3	-854165+6	+653765+2	3000	6000	
MgF	1	+241391+5	+891850+1	+101667-3	-148268+6	+729612+2	500	3000	3
	1	+241381+5	+894563+1	+927083-4	-180145+6	+729614+2	3000	6000	
MgCl	1	+244544+5	+892813+1	+117792-3	-658103+5	+763106+2	500	3000	3
	1	+244535+5	+8938 8+1	+112447-3	-643700+5	+763092+2	3000	6000	
Mg_3N_2	2	+789271+5	+294829+2	+216731-4	+508409+5	+867237+2	1061	2500	12
	2	+789271+5	+294829+2	+216731-4	+508409+5	+867237+2	1061	2500	
$MgAl_2O_4$	2	+128671+6	+368014+2	+639913-2	-978377+6	+116074+3	500	1900	4
	2	+128671+6	+368014+2	+639913-2	-978377+6	+116074+3	500	1900	

TABLE 2. Maximum Fit Error, Expressed as a Percentage of the Original Tabulated Value

Species	$T^{\circ}K$	E_H	$T^{\circ}K$	E_S	$T^{\circ}K$	E_H	$T^{\circ}K$	E_S
Al	4200	.000	4300	.014	5400	.006	4900	.009
Al_2O	0500	.960	0500	.060	4300	.014	5100	.008
Al_2O_3	1200	.053	0700	.119	2400	.001	2800	.057
Al_2O_2	0500	.210	0700	.035	5400	.004	3200	.013
AlCl	2400	.002	1400	.017	4700	.002	5800	.002
$AlCl_3$	2200	.002	0500	.002	4900	.008	4900	.007
$AlCl_2$	1200	.005	0500	.003	4600	.001	4900	.006
$AlCl_3$	0800	.000	0600	.001				
AlF	0500	.110	0500	.005	5300	.002	4800	.002
AlF_3	0800	.046	0800	.020	1100	.020	1400	.016
AlF_3	1900	.002	0800	.001	4700	.010	5200	.008
AlF_2	0500	.073	0500	.013	4400	.001	5400	.005
AlF_2Cl	0500	.062	0500	.013	5900	.004	5900	.005
$AlFCl_2$	0500	.034	2000	.090	5600	.004	5800	.007
AlO	0500	.220	0500	.013	5300	.001	5500	.002
AlOH	0500	.600	0500	.099	5200	.002	4100	.049
AlO_2H	0500	.730	0500	.013	5900	.004	4400	.009
AlOF	0500	.100	0600	.021	5200	.002	4200	.014
AlOCl	0500	.053	1500	.017	6000	.002	4200	.014
AlH	0500	.056	0700	.008	4100	.017	5300	.009
Al			1000	.030	3700	.000	2000	.032
B	2200	.073	0600	.023	4900	.033	4200	.010
B_2	0700	.026	0600	.018	5900	.011	5400	.012
B_2O_2	0500	1.43	0500	.147	4600	.009	4400	.005
B_2O_3	1000	0000	1100	.012	2500	.000	2200	.010
B_2O_3	0500	1.73	0500	.173	4600	.006	5600	.006
BBr	0500	.022	0600	.003	5000	.001	5600	.003
BCl	2500	.033	0500	.014	4400	.017	3300	.011
BCl_3	0500	.327	0500	.019	5000	.007	5400	.005
Be	2200	.065	1900	.021	5000	.041	4100	.022
BeCl	0500	.140	0500	.009	5500	.001	6000	.002
$BeCl_2$	0500	.000	0900	.013				
$BeCl_2$	1500	.052	0700	.016	4100	.009	3500	.007
BeF	0500	.500	0800	.034	5400	.001	4100	.003
BeF_2	0600	.000	0500	.040				
BeF_2	0700	.350	0500	.053	3700	.189	3600	.035
BeFCl	0500	.220	0500	.051	4400	.002	3100	.020
BeO	0500	.780	0500	.052	4000	.002	6000	.002
BeO	2200	.071	0500	.240	2200	.000	4100	.013
BeH	3000	.098	0500	.110	3800	.016	6000	.015
Be	1200	.120	1500	.070	2700	.005	1700	.036

TABLE 2. (Contd.)

Species	$T^{o}K$	E_H	$T^{o}K$	E_S	$T^{o}K$	E_H	$T^{o}K$	E_S
BN	2100	.079	0500	.033	4700	.000	3000	.020
BF	0700	.386	0600	.039	5100	.017	4900	.011
BF_3	0500	.982	0500	.094	4600	.009	5700	.007
BO	0500	1.54	0500	.069	3600	.018	5200	.007
BH	0500	.750	0500	.140	3000	.005	6000	.004
B	0600	1.23	0500	.565	2300	.003	2300	.066
Br_2	1400	.005	1700	.001	4100	.002	3100	.0009
C	3000	.062	0500	.029	6000	.010	3000	.0004
C	1500	.240	0500	.570	2700	.120	2600	.082
C_2	0500	.990	0500	.062	3500	.062	4600	.021
C_2N_2	2500	.120	2200	.210	3900	.028	4500	.007
C_2F_2	0500	.980	0500	.087	5500	.038	3700	.019
C_2H_2	1600	.450	1800	.210	2400	.026	3100	.091
C_2H_4	0600	.002	0600	.018	1300	.015	1000	.012
C_3	0500	1.2	0500	.097	4700	.001	4800	.0006
Cl	0500	.790	0500	.045	5000	.003	5200	.001
Cl_2	1500	.009	1600	.003	4700	.002	4300	.002
ClF	0500	.100	0500	.005	6000	.002	4800	.003
ClO	0500	.150	0500	.010	4300	.002	5200	.003
CN	3000	.056	0500	.018	3000	.030	3000	.003
CF	2600	.043	0500	.038	4800	.023	5500	.046
CF_2	2300	.061	0500	.043	4700	.042	5500	.350
CF_3	2200	.160	0500	.093	4200	.017	5500	.031
CF_4	0900	1.2	0900	.650	5500	.490	5500	.120
CO	0500	1.7	0500	.110	5000	.003	5900	.001
CO_2	0500	1.9	0500	.150	5000	.060	5300	.029
CH	0500	4.7	0500	.170	3000	.003	3900	.0009
CH_2F_2	2500	.150	0500	.230	2800	.001	2700	.008
CH_2	0500	4.1	0500	.310	5600	.000	3900	.0008
CH_2O	0800	.062	0500	.045	1100	.470	1200	.150
CH_3F	2500	.210	0500	.330	3400	.001	4500	.007
CH_4	1000	.047	0600	.010	1200	.012	1900	.003
CHF_3	0500	1.4	0500	.140	3800	.001	3900	.007
Li	1000	.130	0500	.390	1200	.830	1400	1.60
Li	1900	.016	3400	.018	6000	.026	5700	.016
Li_2	2300	.004	2800	.002	4700	.001	5300	.002
Li_2O	1100	.065	0600	.067	3500	.000	1900	.015
Li_2O	0500	.15	0500	.34	5200	.055	3400	.23
Li_2F_2	0500	.110	0500	.021	5900	.004	3900	.006
Li_2Cl_2	0500	.029	2800	.009	5700	.004	4600	.010
LiCl	0500	.057	1400	.003	3600	.002	5100	.002
LiCl	0700	.000	0700	.025	2000	.024	0900	.022
LiF	0500	.170	0500	.012	4600	.002	4100	.002
LiF	1000	.069	1000	.410	1200	.001	2200	.150

TABLE 2. (Contd.)

Species	$T^{o}K$	E_H	$T^{o}K$	E_S	$T^{o}K$	E_H	$T^{o}K$	E_S
LiO	0700	.14	0700	.29	5300	.081	3300	.18
LiOH	0900	.000	1900	.002				
LiH	0500	.074	0500	.220	4000	.13	5000	.73
Mg	3700	.022	3100	.036	5100	.013	4700	.013
$MgAl_2O_4$	0900	.003	0500	.003				
MgCl	2100	.012	0700	.005	4300	.002	5400	.001
$MgCl_2$	0800	.002	0500	.003	1000	.000	1300	.001
$MgCl_2$	1600	.032	1900	.006	4400	.015	6000	.006
MgF	0500	.074	0500	.004	4700	.002	4200	.002
MgF_2	0800	.046	1500	.013	1600	.000	1600	.016
MgF_2	2500	.022	0500	.022	4600	.013	5400	.007
MgFCl	2100	.009	1700	.013	3300	.003	4100	.015
MgO	0500	.110	0500	.006	4900	.003	5700	.002
MgO	1800	.029	2100	.022	2800	.021	3800	.020
MgH	1300	.120	0500	.053	4700	.021	4300	.097
Mg	0800	.006	0800	.025	1700	.051	1400	.042
N	3800	.046	2100	.004	6000	.003	4300	.001
Na	3600	.029	1700	.018	5400	.020	5300	.013
Na_2O	0900	.027	0600	.038				
NaCl	0800	.000	1100	.018				
NaCl	1900	.043	2500	.012	4400	.017	5700	.010
NaF	0700	.110	1200	.026				
NaF	1100	.070	2500	.013	5200	.016	6000	.007
NaOH	1100	.019	0900	.019				
NaOH	3000	.110	0500	.150	4300	.017	6000	.007
NaH	0800	.160	0600	.027	4400	.020	4300	.007
Na	0700	.000	0700	.074				
N_2	0500	1.8	0500	.120	5100	.017	4700	.014
NO	0600	4.0	0500	.330	5000	.014	3000	.002
NO_2	0900	.068	0500	.027	1200	.180	1200	.056
NH	3000	.140	0500	.140	4300	.002	4900	.001
NH_3	1300	.140	1500	.200	3000	.079	1900	.073
F	0500	.160	0500	.010	4400	.002	5000	.002
F_2	0500	.180	0700	.009	4400	.002	5700	.002
F_2CO	0500	.850	0500	.075	4000	.001	2700	.007
FCN	0500	.870	0500	.075	3700	.001	3400	.0005
O	3000	.017	0500	.006	5400	.033	3700	.002
O_2	0600	.180	0500	.017	5900	.009	3000	.002
ONF	0500	.620	0500	.049	4400	.001	4300	.0006
OH	3000	.140	0500	.110	5700	.220	3000	.005
H	2400	.000	1000	.002	4300	.003	5100	.200
H_2	3000	.130	0500	.100	3100	.380	3000	.020
H_2O	3000	.240	0500	.270	5000	.160	5000	.020

TABLE 2. (Contd.)

Species	T^oK	E_H	T^oK	E_S	T^oK	E_H	T^oK	E_S
HBO_2	0500	.206	0500	.170	4000	.010	4700	.008
HBr	0500	2.1	0500	.130	4800	.000	4200	.001
H_3BO_3	3000	.170	0500	.344	4700	.007	4200	.007
HCl	0500	2.10	0500	.140	3700	.003	5100	.001
HCN	1500	.100	0500	.032	2300	.028	3000	1.3
HCO	0500	2.7	0500	.190	3400	.002	3000	.010
HF	3000	.140	0500	.086	3000	.017	3000	.002

RESULTS

The constants are given for the computation of thermodynamic properties for combustion gases at high temperatures by use of the following equations.

$$C_p = a + bT + cT^{-2} \text{ cal/}^oK \tag{1}$$

$$\Delta H^{T_x}_{298.15} = A + \int_{3000}^{T_x} C_p dT \tag{2}$$

$$\Delta H^{T_x}_{298.15} = A + a(T_x - 3000) + \frac{b}{2}(T_x^2 - 3000^2) + c\left[\frac{3000 - T_x}{3000 T_x}\right] \text{cal/mole} \tag{3}$$

$$H^{T_x} = H_{f298.15} + A + \int_{3000}^{T_x} C_p dT$$

$$S^{T_x} = B + \int_{3000}^{T_x} C_p \frac{dT}{T}$$

$$= B + a \ln\left(\frac{T_x}{3000}\right) + b(T_x - 3000) - \frac{c}{2}\left[\frac{1}{T_x^2} - \frac{1}{3000^2}\right] \text{cal/mol - }^oK$$

The standard heats of formation of the combustion species are given in Table 3. Last minute revisions were made to incorporate those values recommended by the JANAF Thermochemical Panel (Ref. 14).

TABLE 3. Standard Heat of Formation of Combustion Species
(Phase 1 = gas, Phase 2, 3 = solid, liquid)

Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol	Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol
Al	1	14	+78.000*	Al	2,3	14	
AlF_2Cl	1	14	-235.0	AlCl	1	14	-11.3
$AlCl_2$	1	14	-78.0	AlOCl	1	14	-55.0
$AlCl_3$	1	14	-139.022	$AlCl_3$	2,3	14	-168.583
AlF	1	14	-61.300	$AlFCl_2$	1	14	-181.8
AlF_3	1	14	-285.448	AlF_3	2,3	14	-356.3
AlF_2	1	14	-157.0	AlOH	1	14	-3.447
AlH	1	14	+61.700	AlN	2	14	-76.000
AlO_2H	1	14	-109.000	AlO	1	14	+17.387
AlN	1	14	+104.5	Mg	2,3	14	-536.000
Al_2Cl_6	1	14	-312.110	Al_2O_3	2,3	14	-400.400
Al_2O	1	14	-39.400	AlOF	1	14	-121.000
Al_2O_2	1	14	-105.280	Al_4C_3	2,3	14	-48.600
AlF_2	1	14	-157.000	B	2,3	14	
B	1	14	+132.618	BFCl	1	14	-76.810
BCl	1	14	+42.5	BOCl	1	14	-84.811
BF_2Cl	1	14	-212.393	$BFCl_2$	1	14	-154.730
BCl_2	1	14	-19.620	BF	1	14	-45.469
BCl_3	1	14	-97.100	BF_2	1	14	-133.843
BOF	1	14	-142.923	BF_3	2,3	14	-270.000
BH	1	14	+114.761	H_3BO_3	1	14	-238.600
HBO_2	1	14	-140.780	BO	1	14	+3.744
$H_2B_2O_4$	1	8	-300.0	BN	2,3	14	-60.3
BN	1	14	+151.748	B_2O_2	1	14	-110.757
B_2	1	14	+199.300	B_2O_3	2,3	14	-305.348
B_2O_3	1	14	-208.268	Be	2,3	14	
B_4C	2,3	14	-12.200	Be_2	1	8	+138.
Be	1	14	+77.922	BeFCl	1	14	-124.000

TABLE 3. (Contd.)

Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol	Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol
BeCl	1	14	+36.989	BeF	1	14	+4.816
$BeCl_2$	1	14	-80.380	BeH	1	14	+77.370
BeF_2	1	14	-182.800	BeO	2,3	14	-143.100
BeO_2H_2	1	14	-156.700	BeO_2H_2	2,3	14	-216.800
BeO	1	14	+30.440	Be_2Cl_4	1	14	-185.000
Be_2C	2,3	14	-22.2	Be_3O_3	1	14	-259.800
Be_2O_2	1	14	-102.400	C	2	14	
Be_3N_2	2,3	14	-132.000	CO_2	1	14	-94.040
C	1	14	-170.890	C_3	1	14	+189.670
CO	1	14	-26.416	CH_2	1	14	+66.000
C_2	1	14	+197.028	CH_4	1	14	-17.889
CH	1	14	+142.100	C_2H_4	1	14	-12.496
CH_3	1	14	+32.000	CH_2O	1	14	-27.400
C_2H_2	1	14	+54.190	Cl_2CO	1	14	-52.400
HCO	1	14	-3.520	HCN	1	14	+31.200
F_2CO	1	14	-150.200	C_2N_2	1	14	+73.840
FClCO	1	14	-106.500	CF	1	14	+76.121
CN	1	14	+94.000	CF_3	1	14	-120.500
FCN	1	14	-25.000	CHF_3	1	14	-162.600
CF_2	1	14	-23.000	CH_3F	1	14	-59.000
CF_4	1	14	-218.000	CCl	1	14	+121.6
CH_2F_2	1	14	-105.500	CCl_4	1	14	-25.500
C_2F_2	1	14	-51.300	H_2	1	14	
H	1	14	+52.102	OH	1	14	+9.330
H_2O	1	14	-57.798	O_2	1	14	
O	1	14	+59.559	N_2	1	14	
N	1	14	+113.054	NO_2	1	14	+8.060
NO	1	14	+21.652	NH_3	1	14	-11.997
NH	1	14	+79.200				

TABLE 3. (Contd.)

Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol	Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol
Cl	1	14	+28.951	Cl_2	1	14	
ClO	1	14	+24.349	ClF	1	14	-13.300
HCl	1	14	-22.060	HF	1	14	-65.140
F	1	14	+18.860	F_2	1	14	
ONF	1	14	-15.650				
Li	1	14	+38.410*	Li	2,3	14	
Li_2C_2	2,3	14	-14.200	Li_2	1	14	+50.400
LiO	1	14	+14.000	Li_2O	2,3	14	-142.600
Li_2O	1	14	-34.100	LiOH	1	14	-57.700
LiH	1	14	+32.100	LiOH	2,3	14	-116.600
LiF	1	14	-79.300	LiF	2,3	14	-145.100
Li_2F_2	1	14	-213.500	LiCl	1	14	-43.800
Li_2Cl_2	1	14	-140.700	LiCl	2,3	14	-97.400
Mg	1	14	+35.330*	Mg	2,3	14	
MgO	1	14	+4.190	MgO	2,3	14	-143.700
$MgCl_2$	1	14	-100.700	$MgCl_2$	2,3	14	-153.220
MgH	1	14	+40.700	MgCl	1	14	+1.000
MgF_2	1	14	-177.000	MgF_2	2,3	14	-262.600
MgFCl	1	14	-138.900	MgF	1	14	-21.000
Na	1	14	+25.755*	Na	2,3	14	
Na_2	1	14	+32.870	NaH	1	14	+29.880
NaO	1	14	+13.200	Na_2O	3,2	14	-100.717
NaCl	1	14	-44.050	NaCl	3,2	14	-98.230
NaF	1	14	-67.000	NaF	2,3	14	-136.300
NaOH	1	14	-55.440	NaOH	2,3	14	-102.240
Si	1	14	+110.000	Si	2,3	14	
Si_2	1	14	+137.000	$SiCl_2$	1	14	-37.660
$SiCl_4$	1	14	-145.700	SiF_4	1	14	-372.900
SiCl	1	14	+48.100	SiF	1	14	+10.300

TABLE 3. (Contd.)

Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol	Species	Phase	Ref	$\Delta H_{f298.15}$ Kcal/mol
SiO_2	1	14	-73.900	SiO_2	2,3	14	-209.863
SiO	1	14	-21.411				
K	1	6	+21.51	K_2	1	6	+30.8
KH	1	6	+30.0	KBr	1	15	-42.5
KF	1	15	-79.8	KCl	1	15	-50.1
CsCl	1	8	-58.200	CsF	1	8	-85.0
CsH	1	6	+29.000	Cs_2	1	6	+27.000
Cs	1	6	+18.830	RbCl	1	15	-49.9
RbH	1	6	+33.3	Rb_2	1	6	+29.6
Rb	1	6	+20.51	RbF	1	8	-87.0
CaO	1	15	-2.0	CaH	1	6	+58.7
Ca	1	6	+46.04	CaCl	1	8	+6.7
CaF	1	8	-9.2				

*This is included as a part of A in the enthalpy and entropy equations and ΔH_f should be taken as zero.

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